Universal free energy correction for the two-dimensional one-component plasma

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The universal finite-size correction to the free energy of a two-dimensional Coulomb system is checked in the special case of a one-component plasma on a sphere. The correction is related to the known second moment of the short-range part of the direct correlation function for a planar system.

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I. INTRODUCTION

Two-dimensional Coulomb systems are models which have attracted some attention. On a two-dimensional manifold, a Coulomb system is a system made of particles interacting through the corresponding Coulomb potential plus perhaps some short-range interaction. In a plane, the Coulomb interaction energy of two particles of charges q and q', separated by a distance r, is defined as $-qq' \ln(r/L)$, where L is some (irrelevant) length.

Some time ago, it has been shown that the free energy of such systems has a universal finite-size correction [1] very similar (except for its sign) to the one which occurs in a system with short-range forces at a critical point [2]: for a finite Coulomb system of characteristic size R, the free energy F has the large-R behaviour

$$\beta F = AR^2 + BR + \frac{\chi}{6} \ln R + \cdots , \tag{1}$$

where β is the inverse temperature. A and B are non-universal constants describing the bulk and boundary contributions, respectively. $(\chi/6)\ln R$ is the universal correction, depending only on the Euler number χ which describes the topology of the manifold on which the system lives. However, the general derivation [1] of (1) had some heuristic features. The purpose of the present paper is to check (1) in the special case of a one-component plasma on the surface of a sphere, by a different method.

The one-component plasma is a system made of one species of point-particles of charge q in a uniform neutralizing background. On a sphere of radius R, the interaction between two particles can be chosen [3,4] as $-q^2 \ln[(2R/L)\sin(\psi/2)]$, where ψ is the angular distance (seen from the sphere centre) between the two particles. There are also particle-background and background-background interactions. A dimensionless coupling constant is $\Gamma = \beta q^2$.

A sphere has no boundaries and its Euler number is $\chi = 2$. Furthermore, for a given particle density, R^2 is proportional to the number of particles N. Thus, expansion (1) becomes

$$\beta F = CN + \frac{1}{6} \ln N + \cdots , \tag{2}$$

where C is a constant. The model is exactly solvable [3] when $\Gamma = 2$ and it can be checked [1] that (2) is obeyed in that case. Also, exact calculations [5] for finite values of N at $\Gamma = 4$ and $\Gamma = 6$ are well fitted by (2).

The present derivation of (2) relies on a recent result [6] about the direct correlation function $c(r)$ of the plane one-component plasma. By a diagrammatic analysis, it has been shown in ref. [6] that the second moment of the short-range part $c_{_{SR}}(r)$ has the simple value

$$n^2 \int c_{_{SR}}(r)\, r^2\, d^2\mathbf{r} = \frac{1}{12\pi}. \tag{3}$$

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A remarkable feature of (3) is its universality, in the sense that it is independent of the coupling constant Γ. It will now be shown how (3) leads to (2). More specifically, we show how (3) implies the finite-size correction to the chemical potential $\mu = \partial F/\partial N$:

$$\beta\mu = \beta\mu_\infty \,+\, \frac{1}{6N} \,+\, \dots \tag{4}$$

This derivation bears some similarity with another one about the two-component plasma [7,8].

II. DENSITY FUNCTIONAL THEORY APPROACH

We consider the OCP of average density n_s on the sphere of radius R (with a corresponding number of particles $N = 4\pi R^2\, n_s$). Introducing the stereographic projection of the sphere onto the plane $\mathcal{P}$ tangent to its south pole (see figure 1), we map the homogeneous OCP on the sphere onto a modified inhomogeneous plasma on the plane, with local particle density

$$n(\mathbf{r}) = n_s\, \left(1 + \frac{r^2}{4R^2}\right)^{-2}. \tag{5}$$

In terms of planar coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, the interaction potential between two particles on the sphere with angular distance ψ_{12} can be written as the sum of the planar two dimensional Coulomb potential $v_p(\mathbf{r},\mathbf{r}') = -q^2\ln[|\mathbf{r}-\mathbf{r}'|/L]$ and one-body terms since:

$$-\ln\left[\frac{2R}{L}\,\sin\left(\frac{\psi_{12}}{2}\right)\right] = -\ln\left[\frac{|\mathbf{r}_1-\mathbf{r}_2|}{L}\right] \,+\, \frac{1}{2}\,\ln\left(1+\frac{r_1^2}{4R^2}\right) \,+\, \frac{1}{2}\,\ln\left(1+\frac{r_2^2}{4R^2}\right). \tag{6}$$

The two one-body terms appearing on the right hand side of eq. (6), as well as the metric, create a central potential and we can consider the projected planar system as a OCP interacting through the standard pair potential v_p, in an external one-body central potential $V_R^N(r)$. The latter acts as a confining mechanism ensuring the proper density given by eq. (5), and its detailed form need not be precised. Without background, the free energy $\mathcal{F}'$ for the set of particles with pair potential v_p can be formally expanded in a Mayer diagrammatic representation [6], with a leading term $(1/2)\int n(\mathbf{r})v_p(\mathbf{r},\mathbf{r}')n(\mathbf{r}')d^2\mathbf{r}\, d^2\mathbf{r}'$ for the excess (over ideal) part of $\mathcal{F}'$. The presence of a neutralizing background cancels this mean-field electrostatic term and the intrinsic free energy functional of the inhomogeneous OCP becomes:

$$\mathcal{F}[n(\mathbf{r})] = \mathcal{F}'[n(\mathbf{r})] - \frac{1}{2}\int n(\mathbf{r})\, v_p(\mathbf{r},\mathbf{r}')\, n(\mathbf{r}')\, d^2\mathbf{r}\, d^2\mathbf{r}'. \tag{7}$$

The local chemical potential reads

$$\mu(\mathbf{r}) = \frac{\delta\mathcal{F}[n]}{\delta n(\mathbf{r})} = \frac{\delta\mathcal{F}'[n]}{\delta n(\mathbf{r})} - \int v_p(\mathbf{r},\mathbf{r}')\, n(\mathbf{r}')\, d^2\mathbf{r}' \tag{8}$$

and the second functional derivative of $\mathcal{F}$ yields:

$$\begin{aligned}
\beta\frac{\delta\mu(\mathbf{r})}{\delta n(\mathbf{r}')} &= \frac{\delta^2\beta\mathcal{F}'[n]}{\delta n(\mathbf{r})\delta n(\mathbf{r}')} - \beta v_p(\mathbf{r},\mathbf{r}') &(9)\\
&= -c(\mathbf{r},\mathbf{r}') + \frac{\delta(\mathbf{r}-\mathbf{r}')}{n(\mathbf{r})} - \beta v_p(\mathbf{r},\mathbf{r}') &(10)\\
&= -c_{_{SR}}(\mathbf{r},\mathbf{r}') + \frac{\delta(\mathbf{r}-\mathbf{r}')}{n(\mathbf{r})}, &(11)
\end{aligned}$$

where the variations of the excess contribution to $\mathcal{F}'$ give rise to the usual direct correlation function [9], having a short-range part given by

$$c_{_{SR}}(\mathbf{r},\mathbf{r}') = c(\mathbf{r},\mathbf{r}') \,+\, \beta v_p(\mathbf{r},\mathbf{r}'). \tag{12}$$

Note that the chemical potential of the OCP on the sphere coincides with $\mu(0)$ for the optimum density profile (5).

Equation (11) emphasizes the short range dependence of the chemical potential on a density perturbation. Consequently, $\mu(0)$ is the same in a finite N-particle OCP in the central potential $V_R^N(r)$ and in the limit $N \to \infty$ with an external potential $V_R^\infty(r)$ ensuring the same density variation around the origin as expression (5), namely:

$$n(\mathbf{r}) = n_s \left(1 - \frac{r^2}{2R^2}\right) + \ldots \tag{13}$$

For the purpose of the present analysis, it is sufficient to truncate (5) after second order in r, as becomes clear below. The knowledge of the finite-size correction to the chemical potential for the OCP on the sphere then amounts to computing the shift $\delta\mu(0)$ induced by switching $V_R^\infty(r)$ starting from the infinite homogeneous planar OCP with density n_s (corresponding to the stereographic projection of the "spherical" plasma in the thermodynamic limit $R \to \infty$). The density variation caused by the addition of $V_R^\infty(r)$ reads $\delta n(\mathbf{r}) \simeq -n_s r^2/(2R^2)$ and induces the shift

$$\beta\,\delta\mu(0) = \int \left[-c_{_{SR}}(\mathbf{r}) + \frac{\delta(\mathbf{r})}{n(\mathbf{r})}\right] \delta n(\mathbf{r})\, d^2\mathbf{r} \tag{14}$$

$$= \frac{n_s}{2R^2} \int c_{_{SR}}(r)\, r^2\, d^2\mathbf{r}, \tag{15}$$

where the direct correlation function to be considered is that of the homogeneous reference planar OCP. From the sum rule (3), we finally obtain:

$$\beta\,\delta\mu(0) = \frac{1}{24\pi n_s R^2} = \frac{1}{6N}, \tag{16}$$

and eq. (4) is recovered.

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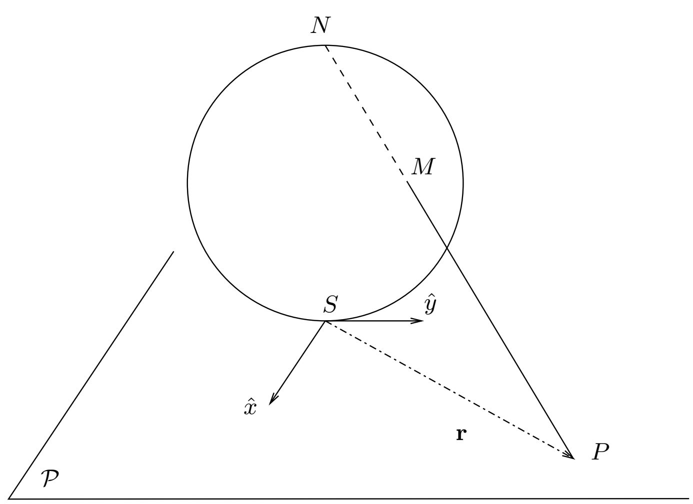

FIG. 1. Stereographic projection from the North pole onto the plane $\mathcal{P}$. A point M on the sphere is projected onto P, with Cartesian coordinates $\mathbf{r}$ ($\mathbf{r} = \mathbf{0}$ at the South pole S).